

Amendments to the Claims

This listing of claims will replace all prior versions and listings of all claims in the application.

Claims 1-17 (cancelled)

18. (New) A method of identifying enzymes with novel catalytic activity, comprising:
 - a) inputting the three dimensional coordinates of a target protein structure with variable residue positions into a computer;
 - b) inserting one or more high energy rotamers into said target protein;
 - c) applying at least one protein design cycle to the target protein structure;
 - d) generating a set of candidate enzymes with putative catalytic activity;
 - e) synthesizing a plurality of said candidate enzymes;
 - f) testing said candidate enzymes for said catalytic activity; and
 - g) selecting at least one candidate enzyme with catalytic activity.
19. (New) A method according to claim 18 wherein said active site domain catalyzes a known enzymatic reaction selected from the group consisting of hydrolases, isomerases, transferases, kinases and phosphatases.
20. (New) A method according to claim 18 wherein said insertion step is done at the same time as said computational step.
21. (New) A method according to claim 18 further comprising applying a second protein design cycle prior to said generating step.
22. (New) A method according to claim 18 in which the protein design cycle comprises protein design automationTM.
23. (New) A method according to claim 18 wherein said protein design cycle comprises a DEE computation.
24. (New) A method according to claim 18 wherein said protein design cycle comprises at least one scoring function.
25. (New) A method according to claim 24 wherein said scoring function is selected from the group consisting of a van der Waals potential scoring function, a hydrogen bond potential scoring function, an atomic solvation scoring function, an electrostatic scoring function and a secondary structure propensity scoring function.
26. (New) A method according to claim 18 wherein said protein design cycle comprises a force field calculation.